

Structural transformations in the system of gypsum-anhydrite during sequential annealing up to 1000 °C

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Abstract

© SGEM2018. The properties of materials obtained during the thermal treatment of gypsum depend on structural defects in the multiphase gypsum-anhydrite system. Analysis of the crystal structures of gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), bassanite ($\text{CaSO}_4 \cdot 0,5\text{H}_2\text{O}$), γ -anhydrite ($\gamma\text{-CaSO}_4$) and natural anhydrite ($\beta\text{-CaSO}_4$) allowed us to identify a common structural motif in each of these structures. This is an irregular hexagon formed by chains of $-\text{Ca}-\text{SO}_4-\text{Ca}-\text{SO}_4-$. During successive thermal transformation of gypsum into anhydrite, this structural motif is retained in all metastable mineral phases with slight distortions in size and shape. Distortions caused by rearrangement of the crystal structure of calcium sulfate minerals create numerous microstresses in the volume of each subsequent newly formed phase. During thermal decomposition of gypsum in the temperature range of 25–500 °C, the sizes of the coherent scattering region (CSR) are successively reduced. At the subsequent increase in the treatment temperature, the dimensions of the CSR begin to increase gradually due to recrystallization and growing domains in crystals of $\beta\text{-CaSO}_4$. A similar tendency is found for structural paramagnetic point defects O^- , O_2^- , SO_3^- . According to electron paramagnetic resonance data, during phase transitions $\text{gypsum} \rightarrow \text{bassanite} \rightarrow \gamma\text{-CaSO}_4 \rightarrow \beta\text{-CaSO}_4$ the concentration of paramagnetic centers increases with temperature growth up to about 400°C and drops at higher temperature. The structural transformations of calcium sulfate minerals are also reflected in surface charge centers. The increase in the concentration of interior structural defects is accompanied by the increase in concentration of surface paramagnetic defects, which is evidenced by EPR spectra. It is shown that structural-phase transformations cause the formation of O^- paramagnetic defects, which can migrate from bulk to the surface and enhance the chemisorption properties, while the formation of O_2^- and SO_3^- defects reduces the concentration of surface active centers.

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Keywords

Anhydrite, Basanite, Gypsum, Paramagnetic center, Thermal transformation

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